Prediction of Residual Stress and Distortion of Ferrous and Non-Ferrous Metals: Current Status and Future Developments

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The quantitative prediction of the consequences of a heat treatment, in terms of microstructure and hardness, residual stresses and distortions, implies a thorough knowledge of the coupled thermal, metallurgical, and mechanical phenomena that occur during the treatment and their modeling. Recent progress made in that field for metallic alloys (steels, aluminum alloys, and titanium alloys) is reviewed through different examples.

1. Introduction

Heat treatments with rapid cooling (quenching) or rapid heating (surface hardening) are difficult to control and optimize. Indeed, it is necessary to control the phase transformations to get the desired mechanical properties and also the thermal gradients in the workpiece either to limit distortions and residual stresses or to get desired residual stress distributions. With this aim, it is essential to understand the processes of internal stress development during the heat treatment. Even if experimental methods for determining residual stresses have made progress, they do not give access to the stress evolutions during the treatment itself. Thus, the only way to get a better knowledge is to model the different phenomena (thermal, metallurgical, and mechanical) that occur during the treatment. Measurements will then be used to validate the calculated results, but only at the end of the treatment.

First approaches in that field concerned the thermal stresses generated during quenching without considering phase transformations.^[1,2] For the last 15 years the main advancements were to take into account microstructural evolutions in the prediction of residual stresses, particularly for steels. A state of the art can be found in several review papers.^[3-6]

In this article, we focus on more recent developments concerning phase transformations and the couplings with the thermomechanical behavior in steels but also for titanium and aluminum alloys. These studies are based on close links between experimental analysis and modeling. Then, we illustrate, through an example, that numerical simulation is a powerful tool to better understand the development of microstructure, internal stresses, and deformations during the treatment. Some limitations and need for future developments will also be addressed.

2. Basis of the Quantitative Prediction of Residual Stresses and Distortions

The different phenomena and couplings that intervene for the prediction of heat treatment residual stresses and distortions are recalled on Fig. $1.^{[7]}$ The temperature gradients in the workpiece induce thermal stresses and phase transformations. The phase transformations through the associated deformations (volume changes and transformation plasticity) and through the induced variations of mechanical properties are also at the origin of internal stresses. They also affect the temperature fields through latent heat and microstructure dependent thermophysical properties. Moreover, stresses and strains affect phase transformations. In addition, chemical composition variations (like those introduced by thermochemical treatments or resulting from solidification) modify the microstructural, thermal and mechanical evolutions. (The deformation energy is generally negligible in heat treatment processes).

Fig. 1 Thermal, metallurgical, and mechanical couplings in heat treatment^[7]

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To fulfill this complete coupling scheme, it is necessary to study and model the metallurgical and mechanical behavior of the material:

- The phase transformations (nature and kinetics) by taking into account the thermal history, the chemical composition, and the stress and strain states,
- The consequences of the phase transformations on the mechanical behavior of the material. Phase transformations generally induce variations in mechanical properties due to the formation of new constituents; moreover, strong couplings between transformation progress and stress can occur (transformation plasticity phenomenon), and
- The heat treatment process, i.e., the thermal gradients in the workpiece during heating and cooling, and in addition the chemical gradients induced by thermochemical treatments (carburizing and carbonitriding).

2.1 Metallurgical and Thermomechanical Behavior of the Material

During the whole heat treatment process (heating and cooling), the material is generally submitted to stresses that can reach its yield stress and to small plastic strains (of the order of the percent). Thus, in the following, we mainly describe the phenomena, their experimental determination, and the modeling under such conditions for the calculation of internal stresses and distortions.

2.1.1 Phase Transformations

Experimental Analysis. For the analysis of a heat treatment process, a thorough knowledge of the phase transformations (mechanisms and kinetics) is necessary. Moreover, the interactions with the stress/strain states must be understood and quantified.

In steels, the austenitization kinetics on heating and the transformation kinetics on cooling are well known through the determination of numerous IT and continuous heating/cooling diagrams.[8,9] Nevertheless, concerning, e.g., tempering, even if the mechanisms of the transformations are well known, $[10]$ only a few studies have clearly quantified the individual kinetics of the different stages of tempering (precipitation of transition carbides, transformation of retained austenite, and transformation of transition carbides into cementite).^[11] Figure 2(a) shows the continuous heating tempering diagram obtained for a 70MC5 steel (H51200 enriched to 0.7% carbon) by using simultaneously dilatometric and resistivimetric measurements to separate the domain of the retained austenite transformation from the transformation of transition carbides into cementite.[12] From these results, the corresponding IT tempering diagram (necessary for the modeling) has been determined by an inverse method (Fig. 2b).

For other metallic alloys, less information can be found about the kinetics of phase transformations. For titanium alloys, precursory work was performed on pseudo α alloys: from dilatometric measurements and microstructural analyses, a CCT diagram for a Ti 6Al5Zr 0.5Mo0.25Si alloy has been obtained.^[13] More recently, anisothermal and isothermal transformation kinetics have been studied for metastable β alloys^[14,15]; particularly, transformation kinetics have been determined by in situ resistivity measurements,[15]; this method is much more sensitive to phase transformation than dilatometry.

Moreover, the mechanisms of the α phase precipitation have been identified.

For high-strength aluminum alloys, the analysis of precipitation during quenching is a more recent preoccupation. $[16]$ The precipitation from the solid solution can occur during quenching when the cooling rates are sufficiently low (the precipitation is heterogeneous at high temperature and becomes homogeneous at lower temperatures). A thorough characterization of the solid solution decomposition during cooling, of the microstructure (nature of precipitates, composition, nucleation sites, etc.) and of the precipitation kinetics has been performed.^[16] Particularly, in situ resistivity measurements at high temperatures (Fig. 3) have given access to the solute depletion of the solid solution and, consequently, to the heterogeneous precipitation kinetics.[17]

Concerning the effect of stress/strain on transformation kinetics, the diffusion-dependent transformations are accelerated by a uniaxial applied stress or a previous deformation of the parent phase due to an increase of nucleation rate.^[18] For transformation with a shear component, it has to be considered that the applied stress brings an additional driving force for the transformation, thus increasing the transformation start temperature on cooling under uniaxial stresses.[19] At the opposite, a relatively small plastic deformation of the parent phase acts as a "resistive" force (due to strain hardening) in the thermodynamic balance and leads to a decrease of the start temperature. But larger plastic strains affect nucleation (role of the defects) and promote the transformation.

We have studied and quantified the mechanisms of these interactions for pearlitic and martensitic transformations of steels^[18,20] and more recently for bainitic transformation.^[21] A work on tempering under tensile stresses^[22] has shown that only the second stage (transformation of retained austenite) is affected by the applied stress: both start temperature and kinetics are modified.

Similar phenomena are encountered in titanium alloys: modification of the $\alpha + \beta \leftrightarrow \beta$ transformation kinetics by a tensile stress (on heating and cooling) has been observed for a Ti6A14V alloy (R56400).[23] More detailed work has been performed to quantify the effect of a plastic deformation of the β phase on the subsequent transformations.[15] Plastic strain of 10% led to a significant acceleration of the transformation kinetics. This has been mainly related to the increase of the grain boundary α phase nucleation rate through quantitative microstructural analysis. Even if such a plastic deformation is much larger than that generally observed in heat treating, these results are essential for taking into account the effects of a thermomechanical treatment on the transformations that occur during heat treatment.

For aluminum alloys, some elements can also be found^[16]; an applied stress or a plastic strain affect the precipitation kinetics, but for the stress and strain levels that develop during quenching these effects are small.

Modeling. For the purpose of calculating heat treatment residual stresses, numerous studies have dealt with the prediction of phase transformation kinetics in steels. In front of the great complexity of industrial steels as far as chemical composition and microstructures are concerned, global approaches have been favored following two main ways: (1) either the modeling of the isothermal kinetics (from IT diagrams) and the

Fig. 2 Continuous heating diagram (a) and IT tempering diagram (b) for 70MC5 steel (H51200 enriched to 0.7% carbon)^[12]

application of an additivity principle or (2) the modeling of anisothermal kinetics from continuous cooling or heating diagrams. A literature review of these different approaches can be found in Ref. 6.

We have developed a model based on isothermal kinetics described by Johnson-Mehl-Avrami type laws.[24,25] It allows us to determine austenitization kinetics on heating and transformation kinetics of austenite into a proeutectoïd constituent, pearlite, bainite, or martensite on cooling. This model takes into account the effect of the austenitic grain size on the transformation kinetics as the effect of a carbon enrichment of austenite due to the ferritic transformation on the subsequent bainitic and martensitic transformations. Moreover, the influence of a stress state has been included as well as the effect of carbon content heterogeneities (as introduced by carburizing or inherited from solidification). Recently, we also included the description of tempering kinetics on heating and self-tempering kinetics on cooling.^[12,26] Figure 4 shows a result of the experimental validation of the model.

A similar modeling approach has been used for the prediction of the precipitation of the α phase from the β phase in a titanium alloy during continuous cooling.[15] In that case, the model takes account of two types of precipitation: (1) the precipitation of α phase at and from grain boundaries (α GB + α WGB) and (2) the precipitation of intragranular α phase $(\alpha$ WI), each being characterized by its own IT diagram. This

Fig. 3 Electrical resistivity variations on isothermal holdings of a 7010 alloy (AlZn6MgCu) after solutionizing at 475 °C and cooling at $50 °C/s^{[17]}$

model predicts correctly the amounts of α phase formed during cooling as illustrated on Fig. 5.

These global approaches are very successful to predict the volume fractions of the different constituents during a complex thermomechanical history of an industrial alloy. But because they do not take into account the nucleation and the growth rates explicitly, they do not allow description of the morphological aspects of the microstructure. Models that include nucleation and growth laws are more and more developed.^[27] Interesting developments are also performed for diffusion controlled transformations based on thermodynamics, mainly in ternary alloys.[28]

For the precipitation in aluminum alloys, such an approach has been developed recently on the basis of the microstructural analysis mentioned above.^[16,29] The model allows description of the kinetics of heterogeneous as well as homogeneous precipitation (at lower temperatures) including nucleation and growth phenomena for isothermal and continuous cooling conditions. An example of simulated results is given in Fig. 6. Detailed analysis can be found in Ref. 30. Moreover, the model allows calculation of the evolution of the matrix composition and of the mean radius of the precipitates, which will affect the mechanical behavior of the alloy.

One can also mention the modeling of γ' precipitation kinetics in nickel-based alloy, $[31]$ including nucleation and coarsening mechanisms to predict volume fraction and precipitate sizes during quenching.

For the models that were developed to take into account the effect of a stress state on the transformation kinetics, a review was given previously.^[32] It can be mentioned that work is in progress to also consider the effects of hot deformation, through dislocation density and grain size, on the subsequent transformations on cooling.[33,34]

2.1.2 Thermomechanical Behavior of the Material

Experimental Analysis. During the heat treatment process, the material undergoes temperature variations and phase transformations. We focus here on the effects of phase transformations on the thermomechanical behavior of the material. The most natural effect is the change in mechanical properties due to the development of a new phase from the parent phase. In addition, we have to consider that the transformation is itself a

Fig. 4 Comparison between calculated transformation kinetics during continuous heating tempering (by using IT diagram of Fig. 2b) and measured ones for 70MC5 steel (H51200 enriched to 0.7% carbon)^[12]

Fig. 5 (a) Calculated kinetics of α precipitation for different cooling rates; beta-CEZ alloy^[15]; (b) final amounts of α phase; comparison between calculation and experiment

Fig. 6 Calculated volume fractions of heterogeneous (a) and homogeneous precipitation (b) at different instants during boiling water quenching for a 7010 alloy (AlZn6MgCu) thick plate^[16,30]

source of deformation and that the stress-transformation interaction may lead to an additional deformation as transformation plasticity.

Numerous experimental studies deal with the mechanical behavior of two constituent stable materials (with no change in volume fractions). The transformation plasticity phenomenon has also been largely studied for diffusion-controlled transformations as well as for shear transformations: the evolutions of transformation plasticity with a constant applied stress are often determined. However, only few studies have reported the evolutions of transformation plasticity with the fraction of the new phase. In steels, results can be found in Refs. 35 and 36. Moreover, the mechanisms of the transformation plasticity have been studied in details to explain these evolutions, particularly for martensitic transformation.^[36] Mainly two mechanisms are considered: the plastic accommodation of the transformation strain (this first mechanism intervenes alone for diffusional transformations) and the orientation of the product phase by the applied stress (due to the shear component of the transformation).

These pieces of information, although absolutely necessary, are not sufficient to completely understand the behavior of the material during a heat treatment process. Indeed, during the

Fig. 7 Stress-strain curves at 450 °C for 27MC5 steel $(H51200)^{[37]}$

Fig. 8 Stress-temperature variations during cooling of a Fe-0.2C steel^[38]

process, the material undergoes simultaneously phase transformations and mechanical evolutions. Thus, the characterization of the mechanical behavior during phase transformations is very important. Typical results obtained for an isothermal bainitic transformation in steel (Fig. 7)^[37] show that the material undergoes softening (low flow stress) as it is deformed during the transformation and that the softening amplitude depends on the deformation rate. Indeed, deformation rate is imposed and the transformation induces its own deformation depending on transformation rate (mainly transformation plasticity). Thus, softening may occur depending on relative values of deformation rate and transformation rate. Similar results have been obtained for a steel deformed during continuous cooling under a ferritic and a pearlitic transformation. $(Fig. 8).^{[38]}$

For other metallic alloys (e.g., titanium alloys), which also present a transformation plasticity deformation, the effect of stress induced transformation has been observed,^[39] and a complex behavior can be obtained at the higher temperatures.

For aluminum alloys, the transformation plasticity phenomenon has not been observed. Of course, the mechanical behavior is modified by precipitation. As an example, even for heterogeneous precipitation a loss of mechanical properties is

Fig. 9 (a) Stress-strain curves obtained after different holding times at 300 °C for a 7010 alloy (AlZn6MgCu) and (b) yield stress evolution vs time for different holding temperatures $[17]$

observed, illustrated on Fig. 9 for isothermal conditions.^[17] The decrease of the yield stress (Fig. 9b) has been related to the precipitation kinetics (characterized by the resistivity variations shown on Fig. 3) and to the solute depletion of the solid solution.

Modeling. The modeling of the thermomechanical behavior of a material undergoing a phase transformation must include the thermoelastic and plastic/viscoplastic behavior of the stable multiphase material and the effect of the phase transformations.

To be able to describe the great complexity of a real material, mainly macroscopic phenomenological behavior laws have been developed.* It is generally assumed that the total strain rate $\dot{\varepsilon}_{ij}^t$ is an addition of different contributions:

$$
\dot{\epsilon}_{ij}^t\ =\ \dot{\epsilon}_{ij}^e + \dot{\epsilon}_{ij}^{th} + \dot{\epsilon}_{ij}^{tr} + \dot{\epsilon}_{ij}^{tp} + \dot{\epsilon}_{ij}^{in}
$$

where

 $\dot{\varepsilon}_{ij}^e$ is the elastic strain rate, which is related to the stress rate by Hooke's law. Young's modulus and Poisson's ratio have to be temperature and microstructure dependent. (Here, "microstructure" means "volume fractions of the different phases").

 $\dot{\epsilon}_{ij}^{\text{th}}$ is the thermal strain rate that takes into account the thermal expansion coefficients of the different phases and their dependence on temperature.

 $\dot{\varepsilon}_{ij}$ is the inelastic strain rate: either the plastic strain rate when no viscous effects are considered or the viscoplastic strain rate. It is calculated by using the classical theory of plasticity or viscoplasticity with the associated hardening rules (isotropic and/or kinematic) or obtained from a micro-macro approach.

All material parameters (yield stress, hardening parameters, strain rate sensitivity, etc.) are to be considered as temperature and microstructure dependent. Mixture rules are generally assumed. In addition, it should be mentioned that taking hardening into account is quite complex when a phase transformation occurs. Models have been proposed to account for some possible "recovery" of strain hardening during a phase transformation, i.e., the new phase "remembers" or not part of the previous hardening.

 ε_{ij}^{tr} is the strain due to the volume change associated with the different phase transformations.

 $\dot{\varepsilon}_{ij}^{\text{tp}}$ is the transformation plasticity strain rate.

Therefore, transformation plasticity deformation rate is considered as an additional strain rate and generally taken as proportional to the transformation rate and to the stress deviator whatever the type of transformation is. Theoritical and micromechanical numerical justifications for this latter assumption have been reviewed in Ref. 32. They rest on the hypothesis that only the first mechanism mentioned above operates. For martensitic transformation, more recent experimental work $[40]$ concluded that this assumption is reasonable within a first approximation, but the model must be refined. Nevertheless, formulation of a macroscopic law for martensitic transformation plasticity in ferrous alloys is still an open question even if micromechanical models have seen outstanding developments.^[41]

Moreover, in the case of chemical composition heterogeneities, its properties depend in addition on local composition. Presently, a dependency with carbon content can be taken into account.[4,6,7,42]

Even though this approach can be considered as crude, it allows to describe rather well the thermomechanical behavior during phase transformation of steels as shown on Fig. 10 for a tensile test performed during continuous cooling. The calculation fits with the experimental stress evolution during cooling with two stress relaxations corresponding to the ferritic and bainitic transformations. The discrepancies on the stress levels have been related to a lack of accuracy in the phase transformation kinetics and in the mechanical properties of the phase mixtures, which depend on temperature and microstructure (volume fractions, which are considered and morphology, which is not taken into account).

Nevertheless, for simpler systems, it is possible to predict the thermomechanical behavior of the material from the deformation mechanisms. For example, in the case of aluminum

^{*}All references on these studies cannot be given here. Most of them can be found in Refs. 6 and 42.

Fig. 10 Stress variations vs time and phase transformation kinetics during continuous cooling for a $27MC5$ steel^[32]

alloys, it has been possible to describe the effect of precipitation on the evolutions of the yield stress by taking into account the softening due to the solute depletion of the solid solution and the hardening due to homogeneous precipitation (by describing the interactions between dislocations and precipitates (amount and mean size).[16]

For the prediction of quenching residual stresses, these variations of the yield stress are then taken into account in the macroscopic behavior law of the material recalled above.^[30] For aluminum alloys, the deformation associated with precipitation (ε_{ij}^{tr}) is negligible because of the very small volume fractions of precipitates, and there is no transformation plasticity (ε_{ij}^{tp}) .

2.2 Heat Treatment Process

Depending on the heat treatment process, it is necessary to describe both the heating process and the cooling process (as in induction, laser, and electron beam hardening) or only the cooling process (in quenching). Moreover, for thermochemical treatments (carburizing and carbonitriding), the diffusion process must be analyzed. We focus hereafter on the cooling stage that is common to all heat treatments

2.2.1 Analysis. If we consider the cooling process, the essential point is the knowledge of the heat transfer between the solid and the quenching medium. The heat transfer mechanisms in vaporizable fluids, which are the most widely used in practice, are complex because different regimens develop film boiling, nucleate boiling, or convection. The main problem comes from the fact that film boiling may be unstable as shown on Fig. 11, and many parameters (temperature and agitation of the bath, state of the surface, geometry of the piece, etc.) can induce destabilization^[43,44] and lead to nonreproducible cooling laws. These fundamental studies have been performed for water,^[43] oils,^[45] and polymer quenchants^[46] and have led to the development of new quenchants providing optimal cooling for metallurgical properties. Presently, work is still performed to get quantitative information parameters that affect the cooling process (measurements of vapor film thickness, flow rates, gaz velocities, etc). $[47]$

Fig. 11 Diagram indicating the possible vaporization regimes during quenching in water at different temperatures of a silver specimen^[43] $(\theta_s$ is surface temperature; θ_L is liquid temperature)

2.2.2 Modeling. The calculation of the temperature fields during heat treatment rests on the solution of heat conduction equation:

$$
\operatorname{div}(\lambda \operatorname{grad} T) + \mathbf{q}^{\text{tr}} + \mathbf{q}^{\text{in}} = \rho c \frac{\partial T}{\partial t}
$$

T is the temperature and t the time. λ , ρ , c are, respectively, thermal conductivity, density and specific heat dependent on temperature and microstructure (generally through mixture rules). These thermophysical properties may also depend on chemical composition. q^{tr} is the power density dissipated by phase transformations. It is related to the transformation rate through:

$$
q^{tr} = \sum \Delta H_k \frac{dy_k}{dt}
$$

where ΔH_k represents the enthalpy variation of the transformation into constituent k and y_k is the volume fraction of constituent k. This term ensures the thermal-metallurgical coupling (Fig. 1).

Heat exchange with the external medium is generally described by a surface heat flux density as boundary condition. For convection on cooling, the heat flux density is given by Newton's law:

\emptyset = h ($T_S - T_{\infty}$)

where h is the heat transfer coefficient, T_S is the surface temperature, and T_{∞} is the temperature of the quenching medium.

Because of the complex heat transfer phenomena evoked above, in most cases, it is not possible to determine directly the heat transfer coefficients (as reviewed in Ref. 48). Their evolutions with surface temperature, position on the surface, etc. are most often determined indirectly by inverse methods based on measured temperature evolutions during cooling (see references in Ref. 6).

Nevertheless, progress is made to solve the coupled heat transfer and convection problems as an example for gas quenching.[49]

On heating, depending on the process, a surface heat source will be considered and described through a surface heat flux density (as for laser heating or electron beam heating), or a volumic heat source will be taken into account (as for induction heating). In this latter case, the solution of electromagnetic equations that allow calculating the eddy current power dissipation qⁱⁿ have to be coupled to the temperature field calculation (see the example in Ref. 50).

The prediction of chemical composition gradients, particularly the carbon content gradients during carburizing, $^{[7]}$ is performed by solving the second Fick's law with appropriate boundary conditions. More general approaches of the coupled diffusion–precipitation phenomena are also developed.^[51]

3. Numerical Simulations

The prediction of residual stresses and distortions implies that the above-mentioned models are included in finite element softwares that solve the whole coupled problem defined in Fig. 1. Presently, besides some in-house softwares (limited to simple geometries but able to treat the whole coupling scheme,^[25] several commercial 2D/3D finite element codes have been and are still developed with this end in view.^[42]

For numerical simulations, the aim is double: they allow a better understanding of the development of microstructures, internal stresses, and deformations during the treatment and, consequently, can lead to a better control of the treatment process. Presently, most of these simulations have been performed for steels and for different heat treatment processes: quenching, surface hardening (induction or laser hardening), case hardening, and even for combined treatments. Numerous examples can be found in the literature.^[6,42]

For other metallic alloys, only a few results are reported and concern quenching residual stresses. Thus, for nickel-based alloys, satisfactory predictions of residual stresses have been obtained in a disc after quenching.^[52] But in that approach, the effect of the microstructural evolutions (modeled elsewhere^[31]) on the thermomechanical behavior law of the material is not taken into account explicitly. This is not the case in the alreadymentioned study on high-strength aluminum alloys $[16]$ in which the thermomechanical behavior law includes precipitation effects. This latter approach has allowed performing a detailed analysis of the consequences of precipitation on the development of residual stresses.^[30]

To illustrate the capabilities of numerical simulations, we have chosen to describe more in detail a study that aims at a better understanding of the development of microstructures and residual stresses during complex heat treatments of steels that combine a thermochemical treatment (carburizing) and a surface-hardening treatment (induction heating + quenching). From the practical point of view, the aim is to find out an optimal heat treatment with regard to mechanical properties and compressive residual stresses of a workpiece.

This study has first needed a full metallurgical^[53] and thermomechanical characterization of the material not only of the base metal (15CD4 steel (K11562)) but also of different carbon-enriched steels. From these studies, the set of input data for the calculation has been established. Moreover, well-controlled heat treatment experiments have been performed on cylinders equipped with thermocouples as well as microstructural analysis and residual stress determinations to validate the numerical simulations.

The calculations have been performed with the in-house software developed for taking into account carbon content gradients.^[25] The investigation concerns a cylinder with 16 mm in diameter and 48 mm in length. The carburizing treatment leads to the measured carbon content profile shown on Fig. 12 (used as an input data for the calculation).

The specimen is induction heated and quenched in salt water at 20 °C: the measured temperature evolutions (Fig. 13) show a mean heating rate of about 250 °C/s at the surface and a maximum temperature of 1000 °C. The temperature fields are calculated with a surface heat flux density boundary condition determined from the measured temperature evolution at 1.5 mm depth by an inverse method.^[54] Temperature evolutions are well described by the calculation, except near the surface over Curie transition, due to the fact that the model does not take into account eddy current losses.

The calculated final microstructure distribution (Fig. 14a) shows that the case-hardened zone is martensitic with an increasing amount of retained austenite as carbon content increases. Moreover, because of the high cooling rates (higher than the critical quenching rate), the heat-affected zone (HAZ), till 4.5 mm depth, undergoes only a martensitic transformation

Fig. 12 Measured carbon content profile after carburizing of 15CD4 steel (K11562)^[54]

Fig. 13 Temperature evolutions at the surface at 1.5 mm below the surface and in the center of a carburized, induction hardened 15CD4 steel (K11562) cylinder

Fig. 14 Final microstructure (a) and hardness (b) distributions in a carburized, induction hardened 15CD4 steel (K11562) cylinder

on cooling. These microstructures are in good agreement with metallographic observations^[55] as well as with the measured retained austenite amounts. The resulting measured and calculated hardness profiles (Fig. 14b) are typical with a plateau at

Fig. 15 Axial stress evolutions during heating and cooling

Fig. 16 Calculated and measured residual stress profiles

the transition between the HAZ and the case-hardened zone and a strong increase of hardness in the case-hardened zone.

The simulated internal stress evolutions (Fig. 15) are to be related to the evolutions of the thermal gradients and to the chronology of the different transformations.[55] It can be noticed that phase transformations generally induce stress relaxations due to the associated volume changes and to transformation plasticity. (A more detailed analysis of these effects can be found in Ref. 32). Moreover, during loading in tension or in compression, the material undergoes plastic strain, the largest amount of it being generated in austenite during cooling. This whole thermomechanical history leads to residual stress profiles (Fig. 16) characterized by high compressive stresses in the surface area: the location of the maximum stress level corresponds to the maximum amount of martensite. But, as the retained austenite amount increases, compressive stresses decrease. The simulation results agree rather well with the experimental ones. It is interesting to notice that the compressive stress levels obtained here are much higher than those obtained after classical carburizing + gas-quenching treatment.

Similar validations have been performed for different cooling conditions. From all the results obtained,^[55] we have concluded that the calculation model and the associated input data are able to predict all the main experimental tendencies as far as microstructures, hardnesses, and residual stresses are concerned. In addition, through numerical experiments, it has been

shown that the level of compressive stresses reached after induction hardening depend highly on the cooling rates. Thus, to achieve high compressive residual stress levels (close to the yield stress of the material), larger cooling rates than the critical quenching rate are necessary, and a critical "mechanical" rate can be defined.^[6]

4. Future Developments

From the results obtained until now in the field of the prediction of heat treatment residual stresses and distortions, several points must be pointed out.

From the point of view of material behavior: the global metallurgical models allow prediction of the phase transformation kinetics for industrial metallic alloys by taking into account the thermal history (heating/cooling), the effects of chemical composition variations, and the effects of stresses as strains. Presently, models that include explicitly nucleation and growth rates are more and more developed for multicomponent alloys. These approaches bring not only information on the amounts of phase formed but also on morphological aspects of the microstructures that are absolutely necessary for the prediction of mechanical properties.

Concerning the thermomechanical behavior of the material and the couplings with the phase transformations, phenomenological behavior laws are able to represent the great complexity of the real behaviors of alloys. Nevertheless, more rigorous approaches, particularly for the prediction of the mechanical behavior of stable multiphase materials (which depends highly on the morphologies and the distributions of the phases), could be better taken into account. In addition, progress is needed in micro-macro approaches that describe the behavior of the transforming material.

For the heat treatment processes, progress to come rests on the couplings between fluid flow and heat transfer to predict more properly the boundary conditions for the thermal problem. This aspect is also related to the development of "new" quenching media, such as gas quenching that leads to less complex heat transfer mechanisms than classical ones. In addition, first steps are performed to model a whole manufacturing process of a workpiece, starting from solidification to forming process and heat treatment.^[56] Work has also been performed to model not only the heat treatment but also to predict the resulting properties of use.^[57]

Concerning industrial applications, numerical simulations are more and more used as help for a better optimization of the heat treatment. Nevertheless, it must be kept in mind that these simulations require numerous input data that can be determined more or less accurately. Thus, although the prediction of microstructures can be considered as satisfactory for residual stresses and distortions, it seems that the most realistic objective of the simulation is to obtain correct trends. For that purpose, more experimental validations at industrial scale and numerical experiments are needed to class the significant parameters for a given process.

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